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| Hexadecanoicacid_methylester**Hexadecanoic acid, methyl ester** | Capture1  (+-)-2-Phenethanamine, 1-methyl-N-vanillyl- |
| 11-OCt**11-Octadecenoic acid, methyl ester** | Capture2 (E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one |
| cis_13_Octadecenoic acid_methyl ester**cis-13-Octadecenoic acid, methyl ester** | Capture31(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans- |

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| Capture4  1-(4-Hydroxy-3-methoxyphenyl)dec-4-en-3-one (6-Shogoal) | 1H Benzo1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-,(4aS-cis)- (alpha-Himachalene) |
| Capture5  1-(4-Hydroxy-3-methoxyphenyl)decane-3,5-dione (gingerdione) | Capture72-Methyl-6-(5-methyl-2-thiazolin-2-ylamino)pyridine |
| Capture61,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z- | Capture83-Decanone, 1-(4-hydroxy-3-methoxy phenyl)- (Paradol) |

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| Capture94aR,5R,9aR)-1,1,4a,8-Tetramethyl-2,3,4,4a,5,6,7,9a-octahydro-1Hbenzo[7]annulen-5-ol (Allohimachalol) | Capture12Caryophyllene |
| Capture1012-Oleanen-3-yl acetate, (3.alpha.)- (beta-Amyrenyl acetate) | Capture13cis-Z-.alpha.-Bisabolene epoxide |
| Capture11Bis(2-ethylhexyl) phthalate | Capture14Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R\*,S\*)]- |

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| Capture15  endo-2-Methylbicyclo[3.3.1]nonane | Capture18 Squalene |
| Capture16 Humulene | Capture19Tetradecanoic acid (myristic acid) |
| Capture17  n-Hexadecanoic acid | |

**Supplementary Figure 9A: 3D and 2D complex structure of binding Interaction between ligand and protein (PDB: 1RW8)**

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| **No interaction. Hexadecanoic acid, methyl ester** | Capture (+-)-2-Phenethanamine, 1-methyl-N-vanillyl- |
| 11-cis-oct**11-Octadecenoic acid, methyl ester** | Capture2 (E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one |
| cis-13 oct**cis-13-Octadecenoic acid, methyl ester** | Capture3  1(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans- |

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| Capture4  1-(4-Hydroxy-3-methoxyphenyl)dec-4-en-3-one (6-Shogoal) | Capture7  1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-,(4aS-cis)- (alpha-Himachalene) |
| Capture5  1-(4-Hydroxy-3-methoxyphenyl)decane-3,5-dione (gingerdione) | **Capture8**  2-**M** **ethyl**-6-(5-methyl-2-thiazolin-2-ylamino)pyridine |
| Capture6  1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z- | Capture9  3-Decanone, 1-(4-hydroxy-3-methoxy phenyl)- (Paradol) |

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| Capture10 4aR,5R,9aR)-1,1,4a,8-Tetramethyl-2,3,4,4a,5,6,7,9a-octahydro-1H-benzo[7]annulen-5-ol (Allohimachalol) | | | | Capture13 Caryophyllene | |
| Capture1112-Oleanen-3-yl acetate, (3.alpha.)- (beta-Amyrenyl acetate) | | | | Capture14 cis-Z-.alpha.-Bisabolene epoxide | |
| Capture12  Bis(2-ethylhexyl) phthalate | | | | Capture15 Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R\*,S\*)]- | |
| Capture16  endo-2-Methylbicyclo[3.3.1]nonane | | | Capture19 Squalene |
| Capture17  Humulene | | | Capture20 Tetradecanoic acid (myristic acid) |
| Capture18  n-Hexadecanoic acid  **Supplementary Figure 9B: 3D and 2D complex structure of binding Interaction between ligand and protein (PDB: 1XO2)** | | | |
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| Hydroxybezoic acid methyl esther**Hexadecanoic acid, methyl ester** | | Capture  (+-)-2-Phenethanamine, 1-methyl-N-vanillyl- | | |
| cis-11**11-Octadecenoic acid, methyl ester** | | Capture2 (E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one | | |
| **NI cis-13-Octadecenoic acid, methyl ester** | | Capture3 1(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans- | | |

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| --- | --- |
| Capture4  1-(4-Hydroxy-3-methoxyphenyl)dec-4-en-3-one (6-Shogoal) | Capture7 1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-,(4aS-cis)- (alpha-Himachalene) |
| Capture5 1-(4-Hydroxy-3-methoxyphenyl)decane-3,5-dione (gingerdione) | Capture8 2-Methyl-6-(5-methyl-2-thiazolin-2-ylamino)pyridine |
| Capture6 1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z- | Capture9 3-Decanone, 1-(4-hydroxy-3-methoxy phenyl)- (Paradol) |

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| Capture10  4aR,5R,9aR)-1,1,4a,8-Tetramethyl-2,3,4,4a,5,6,7,9a-octahydro-1H-benzo[7]annulen-5-ol (Allohimachalol) | Capture13 Caryophyllene |
| Capture1112-Oleanen-3-yl acetate, (3.alpha.)- (beta-Amyrenyl acetate) | Capture14  cis-Z-.alpha.-Bisabolene epoxide |
| Capture12 Bis(2-ethylhexyl) phthalate | Capture15 Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R\*,S\*)]- |

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| Capture16 endo-2-Methylbicyclo[3.3.1]nonane | | | | | | | Capture19 Squalene | |
| Capture17 Humulene | | | | | | | Capture20 Tetradecanoic acid (myristic acid) | |
| Capture18  n-Hexadecanoic acid  **Supplementary Figure 9C: 3D and 2D complex structure of binding Interaction between ligand and protein (PDB: 2O2F)** | | | | | | | | |
| hydroxybenzoic acid methyl esther**Hexadecanoic acid, methyl ester** | **Capture**  (+-)-2-Phenethanamine, 1-methyl-N-vanillyl- | | | |
| 11-cis**11-Octadecenoic acid, methyl ester** | Capture2 (E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one | | | |
| **NI Cis-13-Octadecenoic acid, methyl ester** | Capture3 1(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans- | | | |
| Capture4 1-(4-Hydroxy-3-methoxyphenyl)dec-4-en-3-one (6-Shogoal) | | | | | Capture7  \1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-,(4aS-cis)- (alpha-Himachalene) | | | |
| Capture5  1-(4-Hydroxy-3-methoxyphenyl)decane-3,5-dione (gingerdione) | | | | | Capture8  2-Methyl-6-(5-methyl-2-thiazolin-2-ylamino)pyridine | | | |
| Capture6  1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z- | | | | | Capture9  3-Decanone, 1-(4-hydroxy-3-methoxy phenyl)- (Paradol) | | | |
| Capture10  4aR,5R,9aR)-1,1,4a,8-Tetramethyl-2,3,4,4a,5,6,7,9a-octahydro-1H-benzo[7]annulen-5-ol (Allohimachalol) | | | | | | Capture13 Caryophyllene | |
| Capture1112-Oleanen-3-yl acetate, (3.alpha.)- (beta-Amyrenyl acetate) | | | | | | Capture14  cis-Z-.alpha.-Bisabolene epoxide | |
| Capture12 Bis(2-ethylhexyl) phthalate | | | | | | Capture15 Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R\*,S\*)]- | |
| Capture16 endo-2-Methylbicyclo[3.3.1]nonane | | | | Capture19 Squalene | | | |
| Capture17  Humulene | | | | Capture20Tetradecanoic acid (myristic acid) | | | |
| Capture18  n-Hexadecanoic acid  **Supplementary Figure 9D: 3D and 2D complex structure of binding Interaction between ligand and protein (PDB: 3FZ1)** | | | | | | | |
| hexadecanoic acid methyl esther**Hexadecanoic acid, methyl ester** | | | | | Capture  (+-)-2-Phenethanamine, 1-methyl-N-vanillyl- | | | |
| 11-cis octa**11-Octadecenoic acid, methyl ester** | | | | | Capture2  (E)-1-(4-Hydroxy-3-methoxyphenyl)dec-3-en-5-one | | | |
| cis-13**cis-13-Octadecenoic acid, methyl ester** | | | | | Capture3 1(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans- | | | |
| Capture4  1-(4-Hydroxy-3-methoxyphenyl)dec-4-en-3-one (6-Shogoal) | | | | | | Capture7 1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-,(4aS-cis)- (alpha-Himachalene) | |
| Capture5  1-(4-Hydroxy-3-methoxyphenyl)decane-3,5-dione (gingerdione) | | | | | | Capture8 2-Methyl-6-(5-methyl-2-thiazolin-2-ylamino)pyridine | |
| Capture6  1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z- | | | | | | Capture9 3-Decanone, 1-(4-hydroxy-3-methoxy phenyl)- (Paradol) | |
| Capture10 4aR,5R,9aR)-1,1,4a,8-Tetramethyl-2,3,4,4a,5,6,7,9a-octahydro-1H-benzo[7]annulen-5-ol (Allohimachalol) | | | Capture13Caryophyllene | | |
| Capture1112-Oleanen-3-yl acetate, (3.alpha.)- (beta-Amyrenyl acetate) | | | Capture14cis-Z-.alpha.-Bisabolene epoxide | | |
| Capture12Bis(2-ethylhexyl) phthalate | | | Capture15Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)-6-methylene-, [S-(R\*,S\*)]- | | |
| Capture17endo-2-Methylbicyclo[3.3.1]nonane | | | Capture20Squalene | | |
| Capture18Humulene | | | Capture21Tetradecanoic acid (myristic acid) | | |
| Capture19  n-Hexadecanoic acid | | | | | |

**Supplementary Figure 9E: 3D and 2D complex structure of binding Interaction between ligand and protein (PDB: 4ZY3)**